Spin swapping operator as an entanglement witness for quantum Heisenberg spin-s systems

Guang-Ming Zhang[1,3] and Xiaoguang Wang[2,3]

[1]*Department of Physics, Tsinghua University, Beijing 100084, China;*
[2]*Zhejiang Institute of Modern Physics, Department of Physics, Zhejiang University, Hanzhou 310027, China.*
[3]*Department of Physics and Center of Theoretical and Computational Physics, The University of Hong Kong, Pokfulam Road, Hong Kong, China.*

(Dated: February 1, 2008)

Using the SU(N) representation of the group theory, we derive the general form of the spin swapping operator for the quantum Heisenberg spin-s systems. We further prove that such a spin swapping operator is equal to the spin singlet pairing operator under the partial transposition. For SU(2) invariant states, it is shown that the expectation value of the spin swapping operator and its generalizations, the permutations, can be used as an entanglement witness, especially, for the formulation of observable conditions of entanglement.

PACS numbers: 03.67.-a, 03.67.Mn, 03.65.Ud

I. INTRODUCTION

Entanglement is one of the most intriguing properties of quantum physics and the key ingredient of quantum information and processing. To determine the existence of entanglement, partial transposition of the density matrix is introduced[1, 2]. In 2×2 and 2×3 dimensional Hilbert spaces, the requirement of positive partial transposition (PPT) represents a strong necessary and sufficient criterion for the separability of states, the so-called Peres-Horodecki criterion[1, 2]. A useful entanglement measure for higher dimensions, the negativity, is defined by the sum of absolute value of negative eigenvalues of the partial transposed density matrix[3] though such a criterion of entanglement is no longer sufficient.

Recently it has been realized that symmetries in the mixed states play an important role in characterizing the entanglement properties [4, 5, 6, 7, 8]. For the SU(2) invariant states in dimensions $2 \times L$, $3 \times M$, and 4×4, respectively, the Peres-Horodecki criterion has been proved to be necessary and sufficient[7, 8, 9], where $L = 2j + 1$ with arbitrary spin-j and $M = 2j' + 1$ with j' being integer.

To analyze the general structure of the state space for bipartite $N \times N$ quantum systems, we can regard the subsystems as quantum Heisenberg spin-s systems ($N = 2s + 1$) and transform according to an SU(N) irreducible representation of the group theory. By the requirement of SU(2) invariance, we can substantially reduce the dimensionality of the state space, and the entanglement criteria become easy to be handled analytically.

On the other hand, the entanglement properties in Heisenberg spin systems have received much attention[10]-[37]. For the quantum spin-1/2 system, there is an SU(2) invariant operator, i.e., the swapping operator

$$\mathbf{S}_{i,j} = 2\mathbf{s}_i \cdot \mathbf{s}_j + \frac{1}{2}, \tag{1}$$

which switches the spin states on the sites of i and j. Such a swapping operator satisfies $\mathbf{S}_{i,j}^2 = 1$ and $\mathbf{S}_{i,j}^\dagger = \mathbf{S}_{i,j}$. Therefore, every SU(2) invariant density matrix can be expressed as $\rho_{i,j} = b + c\mathbf{S}_{i,j}$ with suitable real parameters b and c. Actually, one can simply use a single parameter $\langle \mathbf{S}_{i,j} \rangle = \mathrm{Tr}(\rho_{i,j}\mathbf{S}_{i,j})$, which ranges from -1 to 1, to describe these SU(2) invariant states. It is important to notice that for an SU(2) invariant state, the condition $\langle \mathbf{S}_{i,j} \rangle < 0$ has been proved to be *sufficient* and *necessary* for entanglement[38]. There also exists a simple relation between the concurrence[39], quantifying two-qubit entanglement, and the expectation value of the swapping operator with respect to the density matrix $\rho_{i,j}$

$$\mathcal{C}_{ij} = \max(0, -\langle \mathbf{S}_{i,j} \rangle). \tag{2}$$

However, for $s > 1/2$, the operator $2\mathbf{s}_i \cdot \mathbf{s}_j + \frac{1}{2}$ can no longer be regarded as a spin swapping operator, because the SU(2) description is not the faithful fundamental representation for the quantum spin-s operators.

In this paper, based on the SU(N) representation of the group theory, we will first derive the general form of the spin swapping operator for the quantum Heisenberg spin-s system. Then it will be proved that the partial transposed swapping operator is just equal to the singlet pairing operator defined in the tensor product space of the fundamental SU(N) representation and its conjugate one. For an SU(2) invariant spin-s system, we will show that the expectation value of the swapping operator gives rise to the leading contribution to the negativity expressed in terms of the Wigner 6-j symbol. Generalized to the many-body particle states, it will be concluded that the expectation values of the swapping and its generalizations, the permutations, can be used as an entanglement witnesses (EWs) [40, 41, 42], and are useful for the formulation of observable conditions of entanglement.

II. SWAPPING AND SINGLET PROJECTOR FOR QUANTUM HEISENBERG SPIN-s SYSTEMS

A. Spin swapping operator

To describe a spin-s operator quantum mechanically, we use the good quantum numbers: $\mathbf{s}^2 = s(s+1)$ and $s_z = -s, -s+1, ..., s$. The dimensionality of the local Hilbert space is thus $N = 2s+1$. It is natural to introduce an SU(N) fundamental symmetry group with generators in terms of bosons/fermions[43]

$$F_\mu^\nu(i) = a_{i,\mu}^\dagger a_{i,\nu}, \tag{3}$$

where μ and ν denote the spin projection indices from $1, 2, ..., 2s+1$, and i denotes the site. By using the commutation/anticommutation relations,

$$\begin{aligned} [a_{i,\mu}, a_{j,\nu}]_\mp &= \left[a_{i,\mu}^\dagger, a_{j,\nu}^\dagger\right]_\mp = 0, \\ \left[a_{i,\mu}, a_{j,\nu}^\dagger\right]_\mp &= \delta_{i,j}\delta_{\mu,\nu}, \end{aligned} \tag{4}$$

we can prove that the generators satisfy the following commutation relation of the SU(N) Lie algebra[44]

$$\left[F_\mu^\nu(i), F_{\mu'}^{\nu'}(j)\right] = \delta_{i,j}\left(\delta_{\nu,\mu'}F_\mu^{\nu'}(i) - \delta_{\mu,\nu'}F_{\mu'}^{\nu}(i)\right). \tag{5}$$

Accordingly, the corresponding spin operator is expressed as

$$s_i^\alpha = \sum_{\mu,\nu} a_{i,\mu}^\dagger T_{\mu\nu}^\alpha a_{i,\nu}, \tag{6}$$

where T^α ($\alpha = x, y, z$) are the corresponding $N \times N$ matrices for the quantum spin-s operator. We can also prove that the commutation relations of the SU(2) Lie algebra are also satisfied when inserting the expressions of the spin-s operators. In order to fix the magnitude of the quantum spins $\mathbf{s}_i^2 = s(s+1)$, a local constraint $\sum_\mu a_{i,\mu}^\dagger a_{i,\mu} = 1$ has to be imposed as well.

With the help of these SU(N) generators, the general swapping operator between any two sites with N local states each can be constructed as

$$\mathbf{S}_{i,j} = \sum_{\mu,\nu} F_\mu^\nu(i) F_\nu^\mu(j) = \sum_{\mu,\nu} a_{i,\mu}^\dagger a_{j,\nu}^\dagger a_{j,\mu} a_{i,\nu}, \tag{7}$$

which is the *unique* invariant operator under the local SU(N) unitary transformation. In analogy to the Werner states[4], we can define the SU(N)×SU(N) invariant states as follows

$$\begin{aligned} \rho_{i,j} &= p\rho_- + (1-p)\rho_+, \\ \rho_\pm &= \frac{1}{N(N\pm 1)}(1 \pm \mathbf{S}_{i,j}), \end{aligned} \tag{8}$$

where $p = (1 + \langle \mathbf{S}_{i,j}\rangle)/2$ is positive parameter ranging from 0 to 1. Actually, the expectation value of this generalized swapping operator $\langle \mathbf{S}_{i,j}\rangle$ =Tr($\rho_{i,j}\mathbf{S}_{i,j}$), which still ranges from -1 to 1, can be used to describe these SU(N)×SU(N) invariant states. We will further prove that the condition $\langle \mathbf{S}_{i,j}\rangle < 0$ is sufficient for entanglement.

In order to make the swapping operator as a useful EW, it is essential to rewrite this SU(N) swapping operator in terms of cumulants of the original SU(2) spin-s operators. We first notice that

$$\mathbf{s}_i \cdot \mathbf{s}_j = \frac{1}{2}\left[(\mathbf{s}_i + \mathbf{s}_j)^2 - 2s(s+1)\right]. \tag{9}$$

The Hilbert space is thus given by the tensor product space of two quantum spins, and can be decomposed into a sum of irreducible representations in terms of projection operators

$$\mathbf{P}_F = \sum_{M=-F}^{F} |F, M\rangle\langle F, M|, \tag{10}$$

where $F = 0, 1, 2, ..., 2s$ denotes the total spin quantum number, $\mathbf{P}_F$ is the projection operator of the total spin-F channel, and $|F, M\rangle$ corresponds to the irreducible subspace of the tensor product representation for a fixed F. Therefore, a set of relations can be derived as

$$\begin{aligned} (\mathbf{s}_i \cdot \mathbf{s}_j)^n &= \sum_{F=0}^{2s} \lambda_F^n \mathbf{P}_F, \\ \lambda_F &= \frac{1}{2}\left[F(F+1) - 2s(s+1)\right], \end{aligned} \tag{11}$$

where the integer $n = 0, 1, 2, ..., 2s$. Namely, we have a set of equations for the projection operators

$$\begin{aligned} \mathbf{P}_0 + \mathbf{P}_1 + \mathbf{P}_2 + ... + \mathbf{P}_{2s} &= 1, \\ \lambda_0\mathbf{P}_0 + \lambda_1\mathbf{P}_1 + \lambda_2\mathbf{P}_2 + ... + \lambda_{2s}\mathbf{P}_{2s} &= \mathbf{s}_i \cdot \mathbf{s}_j, \\ \lambda_0^2\mathbf{P}_0 + \lambda_1^2\mathbf{P}_1 + \lambda_2^2\mathbf{P}_2 + ... + \lambda_{2s}^2\mathbf{P}_{2s} &= (\mathbf{s}_i \cdot \mathbf{s}_j)^2, \\ &...... \\ \lambda_0^{2s}\mathbf{P}_0 + \lambda_1^{2s}\mathbf{P}_1 + \lambda_2^{2s}\mathbf{P}_2 + ... + \lambda_{2s}^{2s}\mathbf{P}_{2s} &= (\mathbf{s}_i \cdot \mathbf{s}_j)^{2s} \end{aligned} \tag{12}$$

Note that the coefficients in front of the projection operators are of the form λ_F^n, i.e., the corresponding matrix is of the Vandermonde type with the determinant

$$\begin{vmatrix} 1 & 1 & 1 & ... & 1 \\ \lambda_0 & \lambda_1 & \lambda_2 & ... & \lambda_{2s} \\ \lambda_0^2 & \lambda_1^2 & \lambda_2^2 & ... & \lambda_{2s}^2 \\ .. & .. & .. & ... & .. \\ \lambda_0^{2s} & \lambda_1^{2s} & \lambda_2^{2s} & ... & \lambda_{2s}^{2s} \end{vmatrix} = \prod_{k<l}(\lambda_k - \lambda_l). \tag{13}$$

By using the property of the Vandermonde determinant, we can obtain the general expression for the projection operators in terms of the SU(2) spin-s operators

$$\mathbf{P}_F = \prod_{\substack{k=0 \\ \neq F}}^{2s} \left[\frac{\mathbf{s}_i \cdot \mathbf{s}_j - \lambda_k}{\lambda_F - \lambda_k}\right]. \tag{14}$$

Moreover, the general SU(N) invariant swapping operator can thus be expressed as

$$\mathbf{S}_{i,j} = (-1)^{2s} \sum_{F=0}^{2s} (-1)^F \mathbf{P}_F = \prod_{\substack{k=0 \\ \neq F}}^{2s} \left(\frac{\mathbf{s}_i \cdot \mathbf{s}_j - \lambda_k}{\lambda_F - \lambda_k} \right). \quad (15)$$

Namely, the general spin swapping operator is written as a linear combination of all projection operators for the spin-F channels with alternating sign, and $\mathbf{S}_{i,j}$ is symmetric for integer spins and antisymmetric for the odd-half integer spins when interchanging the spin states on the sites of i and j. Similar expressions for the projections had appeared in the literature[45, 46].

As examples, the first four expressions of the general swapping operators are explicitly written as

i). For $s = 1/2$, the above expression gives rise to

$$\mathbf{S}_{i,j} = 2\mathbf{s}_i \cdot \mathbf{s}_j + \frac{1}{2}, \quad (16)$$

which is invariant under the SU(2) unitary transformation.

ii). For $s = 1$, the swapping operator is

$$\mathbf{S}_{i,j} = (\mathbf{s}_i \cdot \mathbf{s}_j)^2 + (\mathbf{s}_i \cdot \mathbf{s}_j) - 1, \quad (17)$$

which is invariant under the SU(3) unitary transformation.

iii). For $s = 3/2$, the swapping operator takes the form

$$\begin{aligned} \mathbf{S}_{i,j} &= \frac{2}{9} (\mathbf{s}_i \cdot \mathbf{s}_j)^3 + \frac{11}{18} (\mathbf{s}_i \cdot \mathbf{s}_j)^2 \\ &\quad - \frac{9}{8} (\mathbf{s}_i \cdot \mathbf{s}_j) - \frac{67}{32}, \end{aligned} \quad (18)$$

which is invariant under the SU(4) unitary transformation.

iv). For $s = 2$, the swapping operator is expressed as

$$\begin{aligned} \mathbf{S}_{i,j} &= \frac{1}{36} (\mathbf{s}_i \cdot \mathbf{s}_j)^4 + \frac{1}{6} (\mathbf{s}_i \cdot \mathbf{s}_j)^3 \\ &\quad - \frac{13}{36} (\mathbf{s}_i \cdot \mathbf{s}_j)^2 - \frac{5}{2} (\mathbf{s}_i \cdot \mathbf{s}_j) - 1. \end{aligned} \quad (19)$$

which is invariant under the SU(5) transformation.

Thus, the expectation value of the swapping operator $\langle \mathbf{S}_{i,j} \rangle$ can be written in terms of the cumulants of the quantum spin-s correlators. In solid state physics, the swapping operator is used to represent the generalized SU(N) invariant quantum Heisenberg spin-s model, i.e., $H = J \sum_{\langle i,j \rangle} \mathbf{S}_{i,j}$, to describe the possible nearest neighbor couplings of magnetic spin-s moments. In one dimension, there exists so-called Bethe ansatz exact solution[47, 48]. For the antiferromagnetic coupling ($J > 0$), the ground state is a singlet with spin *gapless* excitations[49].

B. Spin singlet projector

Among all the projection operators, the singlet projector represents a maximally entangled state, and its expectation value in some cases has been used for formulation of necessary and sufficient conditions of entanglement. In terms of original SU(2) spin-s operators, we have

$$\mathbf{P}_{ij} = \mathbf{P}_{F=0} = \prod_{k=1}^{2s} \left[1 - 2 \frac{\mathbf{s}_i \cdot \mathbf{s}_j + s(s+1)}{k(k+1)} \right]. \quad (20)$$

The corresponding spin singlet state can be projected onto the angular momentum singlet state

$$|0,0\rangle = \frac{1}{\sqrt{2s+1}} \sum_{m=-s}^{s} (-1)^{s-m} |s,m\rangle_i \otimes |s,-m\rangle_j. \quad (21)$$

In particular, the first four expressions for the singlet projectors can be explicitly written as

i). For $s = 1/2$, the singlet operator is

$$\mathbf{P}_{ij} = \frac{1}{4} - \mathbf{s}_i \cdot \mathbf{s}_j. \quad (22)$$

Then, the swapping operator $\mathbf{S}_{i,j}$ and the singlet projection operator $\mathbf{P}_{i,j}$ are not independent. They have the following relation $\mathbf{S}_{i,j} = (1 - 2\mathbf{P}_{i,j})$. The entanglement criterion for the SU(2) invariant states $\langle \mathbf{S}_{i,j} \rangle < 0$ implies that $\langle \mathbf{P}_{i,j} \rangle > 1/2$.

ii). For $s = 1$, the singlet projection is given by

$$\mathbf{P}_{i,j} = \frac{1}{3} \left[(\mathbf{s}_i \cdot \mathbf{s}_j)^2 - 1 \right]. \quad (23)$$

iii). For $s = 3/2$, the singlet projection is written as

$$\begin{aligned} \mathbf{P}_{i,j} &= \frac{33}{128} + \frac{31}{96} \mathbf{s}_i \cdot \mathbf{s}_j \\ &\quad - \frac{5}{72} (\mathbf{s}_i \cdot \mathbf{s}_j)^2 - \frac{1}{18} (\mathbf{s}_i \cdot \mathbf{s}_j)^3. \end{aligned} \quad (24)$$

iv). For $s = 2$, the singlet projection is expressed as

$$\begin{aligned} \mathbf{P}_{i,j} &= -\frac{1}{3} \mathbf{s}_i \cdot \mathbf{s}_j - \frac{17}{180} (\mathbf{s}_i \cdot \mathbf{s}_j)^2 \\ &\quad + \frac{1}{45} (\mathbf{s}_i \cdot \mathbf{s}_j)^3 + \frac{1}{180} (\mathbf{s}_i \cdot \mathbf{s}_j)^4. \end{aligned} \quad (25)$$

All these singlet projectors display *uniform* SU(2) invariance superficially, but it will be further proved that a non-uniform higher symmetry is associated with each singlet projector.

Therefore, the expectation value of the singlet projectors can be also expressed in terms of the cumulants of the quantum spin-s correlators. In solid state physics, the singlet pairing projection is also used to represent another type of the generalized quantum Heisenberg spin-s model, i.e., $H = -J \sum_{\langle i,j \rangle} \mathbf{P}_{i,j}$, to describe the nearest neighbor couplings of the magnetic spin-s moments. In one dimension, an exact solution has been found based on Temperley-Lieb algebra[45]. Moreover, in the case of $J > 0$, the ground state is a dimerized-like singlet state with *gapful* spin excitations[46].

C. Relation between swapping and singlet pairing operators

According to group theory[44], for an SU(N) Lie group with $s > 1/2$, two kinds of spinors (upper and lower) can actually be defined. The lower spinor transforms according to the SU(N) fundamental representation, while the upper spinor transforms according to the SU(N) conjugate representation. More importantly, the conjugate representation is in general independent of the fundamental representation. Only for $s = 1/2$ ($N = 2$), due to the presence of an additional *particle-hole* symmetry, these two representations are equivalent to each other[44].

The generators of the SU(N) conjugate representation is defined by[43]

$$\widetilde{F}_{\mu}^{\nu}(i) = a_{i,\nu}^{\dagger} a_{i,\mu}, \tag{26}$$

where μ and ν denote the spin projection indices from $1, 2, ..., 2s + 1$, and i denotes the site. By using the commutation/anticommutation relations for bosons/fermions, we can prove the following commutation relation

$$\left[\widetilde{F}_{\mu}^{\nu}(i), \widetilde{F}_{\mu'}^{\nu'}(j)\right] = \delta_{i,j}\left(\delta_{\nu,\mu'}\widetilde{F}_{\mu}^{\nu'}(i) - \delta_{\mu,\nu'}\widetilde{F}_{\mu'}^{\nu}(i)\right), \tag{27}$$

which also forms an SU(N) Lie algebra. Consider two quantum spins, i.e., the bipartite system. With the help of generators of the SU(N) fundamental and its conjugate representations, a singlet pairing operator between two sites i and j can be constructed as

$$\mathbf{P}'_{i,j} = \sum_{\mu,\nu} F_{\mu}^{\nu}(i)\widetilde{F}_{\nu}^{\mu}(j) = \sum_{\mu,\nu} a_{i,\mu}^{\dagger} a_{j,\mu}^{\dagger} a_{j,\nu} a_{i,\nu}, \tag{28}$$

which is the unique SU(N)$\times\widetilde{\mathrm{SU}(N)}$ invariant operator and is positive with norm $d = 2s+1$. The corresponding maximally entangled state is expressed as

$$|0,0\rangle' = \frac{1}{\sqrt{2s+1}} \sum_{m=-s}^{s} |s,m\rangle_i \otimes |s,m\rangle_j. \tag{29}$$

In analogy to the so-called symmetric/isotropic states [5], we can define the SU(N)$\times\widetilde{\mathrm{SU}(N)}$ invariant states, and every SU(N)$\times\widetilde{\mathrm{SU}(N)}$ invariant state can be expressed as $\rho_{i,j} = b' + c'\mathbf{P}'_{i,j}$ with suitable real parameters b' and c', or in terms of a convex combination of two minimal projections

$$\rho_1 = \frac{1}{2s+1}\mathbf{P}'_{i,j}, \rho_2 = \frac{1}{4s(s+1)}(1-\rho_1). \tag{30}$$

Now we are in the position to establish the relation between the general spin swapping and the singlet pairing operators. In studying entanglement a powerful tool, the operation of partial transposition, has been introduced[1, 2]. The partial transposition of an operator in the $N \times N$ product space of a bipartite system is defined in a product basis by transposing only the indices belonging to the second basis and keeping those pertaining to the first basis. When applying such a partial transposition operation to the SU(N)$\times\widetilde{\mathrm{SU}(N)}$ invariant singlet pairing operator, we find a very important relation

$$\begin{aligned} \mathbf{P}'_{i,j} &= \sum_{\mu,\nu} a_{i,\mu}^{\dagger} a_{j,\mu}^{\dagger} a_{j,\nu} a_{i,\nu}, \\ &\Leftrightarrow \sum_{\mu,\nu} a_{i,\mu}^{\dagger} a_{j,\nu}^{\dagger} a_{j,\mu} a_{i,\nu} = \mathbf{S}_{i,j}. \end{aligned} \tag{31}$$

Namely, the partial transpose of the SU(N)$\times\widetilde{\mathrm{SU}(N)}$ invariant singlet pairing operator is *exactly* equivalent to the uniform SU(N)$\times$SU(N) invariant swapping operator. The inverse statement also holds true. This is one of the main results of our present paper. Actually a similar relation exists between the Werner states and symmetric/isotropic states[6].

Moreover, Breuer has convincingly demonstrated that [8] the partial transposition is *equivalent* to the partial time reversal transformation of the quantum Heisenberg spin-s operator. Under such a partial time reversal transformation, the corresponding SU(N)$\times\widetilde{\mathrm{SU}(N)}$ invariant singlet pairing state *exactly* transforms into the singlet state in the fundamental SU(N) representation

$$\begin{aligned} |0,0\rangle' &= \frac{1}{\sqrt{2s+1}} \sum_{m=-s}^{s} |s,m\rangle_i \otimes |s,m\rangle_j \\ &\Leftrightarrow \frac{1}{\sqrt{2s+1}} \sum_{m=-s}^{s} (-1)^{s-m} |s,m\rangle_i \otimes |s,-m\rangle_j, \end{aligned}$$

implying that the spin singlet projection state defined in the SU(N) fundamental representation equal to the spin singlet pairing state defined by the product of the SU(N) fundamental and its conjugate representations. Moreover, the singlet projection operator $\mathbf{P}_{i,j}$ shares the same symmetry of SU(N)$\times\widetilde{\mathrm{SU}(N)}$ displayed by the singlet paring operator.

III. SWAPPING OPERATOR AND ITS GENERALIZATIONS AS ENTANGLEMENT WITNESSES

Formulation of different criteria, which allows one to distinguish in experiment entangled and disentangled states, is one of the most important issues in the field of foundations of quantum physics and quantum information processing. The corresponding studies lead to quick development of the theory of EWs [50]-[58]. An entanglement witness [40, 41, 42] is a Hermitian operator with a key property that its expectation value on a separable state is always larger or equal to zero. So, if the expectation value on a state is less than zero, then the corresponding state is entangled.

A. Swapping and negativity

Consider a many-body state, we first study the two-spin state, and the generalization to a many particle spin state is straightforward. Swapping operator exhibits a uniform SU(N) symmetry, and we may exploit it to detect entanglement in a quantum Heisenberg spin-s system. The action of the swapping on a product state is given by

$$\mathbf{S}_{ij}|\phi_i\rangle \otimes |\phi_j\rangle = |\phi_j\rangle \otimes |\phi_i\rangle. \tag{32}$$

A separable (non-entangled) two-particle reduced density matrix ρ_{ij} is introduced as

$$\rho_{ij} = \sum_k p_k |\phi_i^k\rangle\langle\phi_i^k| \otimes |\phi_j^k\rangle\langle\phi_j^k|, \tag{33}$$

where the coefficients p_k are positive real numbers, satisfying $\sum_k p_k = 1$, and $|\phi_i^k\rangle$ is the state for the i-th particle. Evaluating the expectation value of $\mathbf{S}_{i,j}$ on this separable state, we find that

$$\begin{aligned}\langle\mathbf{S}_{i,j}\rangle =&\mathrm{Tr}(\mathbf{S}_{i,j}\rho_{ij})\\ =&\mathrm{Tr}\left(\sum_k p_k |\phi_j^k\rangle\langle\phi_i^k| \otimes |\phi_i^k\rangle\langle\phi_j^k|\right)\\ =&\sum_k p_k |\langle\phi_i^k|\phi_j^k\rangle|^2 \geq 0.\end{aligned} \tag{34}$$

This inequality is fulfilled for all separable states, and it directly follows that any state with $\langle\mathbf{S}_{i,j}\rangle < 0$ is sufficiently entangled. In other words, the swapping has the property of an EW and the following theorem holds true.

Proposition I: If the expectation value of $\mathbf{S}_{ij}$ *on all separable states is larger or equal to zero, then the inequality*

$$\langle\mathbf{S}_{ij}\rangle < 0 \tag{35}$$

implies that the corresponding quantum state is sufficiently entangled.

For an SU(2) invariant state of spin-1/2 systems, the condition $\langle\mathbf{S}_{i,j}\rangle < 0$ is sufficient and necessary for entanglement [38]. We would like to emphasize that the above theorem is not restricted to the spin systems, but also applicable to any composite systems consisting two identical subsystems, e.g., two d-level systems and two identical infinite-dimensional systems. It is interesting to notice that Horodecki *et al* had found that any *permutation of indices* of a density matrix leads to the separability criterion[60]. Here our considerations focus on the swapping of the quantum spin states on two different sites. What is more, our analyses have shown that *not* all such permutations can be regarded as a separability criterion.

Swapping operator has appeared in the expression of the concurrence in spin-1/2 systems, and it can be expected to manifest itself in the negativity expression of the SU(2)-invariant states for arbitrary quantum spin-s systems. For an SU(2) invariant state, the density operator can be written as a linear combination of the projection operators,

$$\rho = \frac{1}{2s+1}\sum_{F=0}^{2s}\frac{\alpha_F}{\sqrt{2F+1}}\mathbf{P}_F, \quad \alpha_F = \frac{2s+1}{\sqrt{2F+1}}Tr(\rho\mathbf{P}_F), \tag{36}$$

where F is the quantum number of the total angular momentum ($\mathbf{s}_i$+$\mathbf{s}_j$). After partial transposition with respect to the second spin, the transposed density matrix still has an SU(2) symmetry, and can be written as [7]

$$\rho^{T_2} = \frac{1}{2s+1}\sum_{K=0}^{2s}\frac{\alpha'_K}{\sqrt{2K+1}}\mathbf{P}'_K, \tag{37}$$

where K is the quantum number of another angular momentum composed of $\mathbf{s}_i$ and $\mathbf{s}_j$: $K_{ij}^x = s_i^x - s_j^x$, $K_{ij}^y = s_i^y + s_j^y$, $K_{ij}^z = s_i^z - s_j^z$. As shown by Breuer [8], a relation between the coefficient vectors $\vec{\alpha}'$ and $\vec{\alpha}$ can be established

$$\begin{aligned}\vec{\alpha}' &= \mathbf{\Theta}\vec{\alpha},\\ \mathbf{\Theta}_{FK} &= \sqrt{(2F+1)(2K+1)}\begin{pmatrix} s & s & F\\ s & s & K\end{pmatrix},\end{aligned} \tag{38}$$

where $\vec{\alpha} = (\alpha_0, \alpha_1, ..., \alpha_{2s})^T$, $\vec{\alpha}' = (\alpha'_0, \alpha'_1, ..., \alpha'_{2s})^T$, and $\mathbf{\Theta}_{FK}$ is given by the Wigner 6-j symbol [59]. From Eq. (37), the negativity of the corresponding density matrix is then calculated as

$$\mathcal{N} = \frac{1}{2s+1}\sum_{K=0}^{2s-1}\max\left(0, -\sqrt{2K+1}\sum_{F=0}^{2s}\mathbf{\Theta}_{KF}\alpha_F\right), \tag{39}$$

where the last term in the K summation does not contribute to the negativity.

For an $s = 1/2$ bipartite system, the above negativity gives rise to $\mathcal{N}$ =max$(0, -\langle\mathbf{s}_i{\cdot}\mathbf{s}_j\rangle)$. However, for the $s = 1$ bipartite system, the corresponding negativity is given by

$$\begin{aligned}\mathcal{N} &= \frac{1}{3}\max(0, -\langle\mathbf{s}_i{\cdot}\mathbf{s}_j\rangle - \langle(\mathbf{s}_i{\cdot}\mathbf{s}_j)^2\rangle)\\ &+\frac{1}{2}\max(0, \langle(\mathbf{s}_i{\cdot}\mathbf{s}_j)^2\rangle - 2).\end{aligned} \tag{40}$$

The expectation values of the swapping operators have included in the above expressions. From the properties of the Wigner 6-j symbol [59], the first term in the summation over K is given by

$$\Theta_{0F} = (-1)^{2s+F}\frac{\sqrt{2F+1}}{2s+1}. \tag{41}$$

Then, the leading term in the negativity expression can be evaluated as

$$\begin{aligned}&\frac{1}{2s+1}\max\left(0, (-1)^{2s+1}\sum_{F=0}^{2s}(-1)^F\mathrm{Tr}(\rho\mathbf{P}_F)\right)\\ =&\frac{1}{2s+1}\max\left(0, -\langle\mathbf{S}\rangle\right).\end{aligned} \tag{42}$$

Therefore, being as an EW, the swapping operator has been included in the expression of negativity as the leading contribution for arbitrary quantum spin-s systems. Actually, this is also one of the main results of the present paper.

As an application of the above result, for the following SU(2) invariant pure state

$$\rho = \frac{1}{4s+1}\mathbf{P}_{2s-1}, \tag{43}$$

the expectation value of the swapping operator on this state is found to be -1, where only the term containing swapping operator survives. Thus, the negativity for this particular pure state is $1/(2s+1)$, and the corresponding state is entangled.

B. Generalization of swapping

A natural generalization of the swapping is the permutation $\mathbf{R}$. The action of $\mathbf{R}$ on a product state is given by

$$\mathbf{R}|\phi_1\rangle\otimes|\phi_2\rangle\otimes\ldots\otimes|\phi_N\rangle = |\phi_{i_1}\rangle\otimes|\phi_{i_2}\rangle\otimes\ldots\otimes|\phi_{i_N}\rangle \tag{44}$$

All $N!$ permutations form a permutation group. We now evaluate $\mathbf{R}$ on a separable state. A N-particle density matrix ρ is separable (non-entangled) if it can be decomposed into

$$\begin{aligned}\rho = \sum_k p_k |\phi_1^k\rangle\langle\phi_1^k| \otimes\cdots\otimes |\phi_i^k\rangle\langle\phi_i^k|\otimes\cdots \\ \otimes|\phi_j^k\rangle\langle\phi_j^k|\otimes\cdots\otimes|\phi_N^k\rangle\langle\phi_N^k|,\end{aligned} \tag{45}$$

where the coefficients p_k are positive real numbers satisfying $\sum_k p_k = 1$, and $|\phi_i^k\rangle$ is the state for the i-th particle. For some permutation operators, such as swaps, we can prove that the corresponding expectation value on a separable state is always large or equal to zero, we thus conclude that these permutation operators can also be viewed as EWs. Then, we have following conclusion.

Proposition II: If the expectation value of permutation $\mathbf{R}$ *on all separable states is large or equal to zero, then the inequality*

$$\langle\mathbf{R}\rangle < 0 \tag{46}$$

implies that the corresponding quantum state is sufficiently entangled.

For $N = 2$, the permutation group contains a swap and an identity. For $N = 3$, the permutation group contains 6 elements, and three different swappings, namely, $\mathbf{S}_{12}$, $\mathbf{S}_{13}$, and $\mathbf{S}_{23}$ are EWs. For $N = 4$, there are 24 elements, and except swappings, there are other permutations can be viewed as EWs, e.g., $\mathbf{S}_{12}\mathbf{S}_{34}$, $\mathbf{S}_{13}\mathbf{S}_{24}$, and $\mathbf{S}_{14}\mathbf{S}_{23}$. Among them, the operator $\mathbf{S}_{14}\mathbf{S}_{23}$ can be viewed as an mirror reflection. Furthermore, any superpositions of the EWs $\sum_{k=1}^{M} c_k\mathbf{P}_k$ with c_k being positive can also be viewed as new EWs.

C. Singlet projector as an EW

For the SU(2) invariant states, the negativity for the spin-1 bipartite systems has been obtained as

$$\mathcal{N} = \frac{1}{2}\max\left(0, 3\langle\mathbf{P}_{i,j}\rangle - 1\right) + \frac{1}{3}\max\left(0, -\langle\mathbf{S}_{ij}\rangle\right). \tag{47}$$

We have observed that the inequality $\langle\mathbf{P}_{i,j}\rangle > 1/3$ also implies that the corresponding state is entangled. As we have shown in previous section, the spin swapping operator and singlet projector are independent though the partial transposition is related to them. For the SU(2)-invariant state, there can be two *different* sufficient entanglement conditions for the spin-1 bipartite systems: one is $\langle\mathbf{S}_{i,j}\rangle < 0$ and another is $\langle\mathbf{P}_{i,j}\rangle > 1/3$. In fact, we can prove a more general theorem for arbitrary quantum spin-s systems.

Proposition III: If the expectation value of the singlet projector satisfies

$$\langle\mathbf{P}_{i,j}\rangle > \frac{1}{2s+1}, \tag{48}$$

the corresponding many-body quantum spin state is sufficiently entangled.

Proof: A singlet state is given by

$$|\Psi_s\rangle = \frac{1}{\sqrt{2s+1}}\sum_{m=-s}^{s}(-1)^{s-m}|s,m\rangle\otimes|s,-m\rangle, \tag{49}$$

and the singlet projector can be expressed as $P_0 = |\Psi_s\rangle\langle\Psi_s|$. A product state can always be written as

$$|\Phi\rangle = |\Phi_1\rangle\otimes|\Phi_2\rangle = \sum_{m,m'} a_m b_{m'}|s,m\rangle\otimes|s,m'\rangle, \tag{50}$$

where $\sum_m |a_m|^2 = \sum_m |b_m|^2 = 1$. Then the expectation value $\langle P_0\rangle$ with respect to this product state is found to be

$$\langle\mathbf{P}_{ij}\rangle = \frac{1}{2s+1}\left|\sum_{m=-s}^{s}(-1)^{s-m}a_m b_{-m}\right|^2 \le \frac{1}{2s+1}, \tag{51}$$

where the inequality follows from the Schwatz inequality and the normalization conditions. We may easily extend the above inequality to the case of any separable state. For an arbitrary separable state $\rho_{sep} = \sum_k p_k\rho_k$ with ρ_k being the product state. The expectation value of $\mathbf{P}_{ij}$ satisfies the inequality

$$\langle\mathbf{P}_{ij}\rangle = \mathrm{Tr}(\mathbf{P}_{ij}\rho) = \sum_k p_k Tr(\mathbf{P}_{ij}\rho_k) \le \frac{1}{2s+1}, \tag{52}$$

where we have used Eq. (51). Therefore, the theorem has been proved, and at the same time the operator $\left(\mathbf{P}_{ij} - \frac{1}{2s+1}\right)$ is another class of EW.

D. Relations with other EWs

The quantum spin Hamiltonians have already been used as EWs to detect entanglement [50, 51]. Here, we would like to study the relations among them. Let us consider the following Hamiltonian

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_{i,j}, \tag{53}$$

which is a sum of all different swaps on the nearest neighbor sites. We know that every expectation value of each swap on a separable state is large or equal to zero. Then, the expectation value of the Hamiltonian on a separable state satisfies $\langle H \rangle \geq 0$. Therefore, the Hamiltonian is regarded as an EW too. For any eigenstate, if the eigenenergy is less than zero, the many-body state must be entangled. We see that a new EW was constructed by superpositions of swaps. In fact, any superposition of swaps with positive coefficients are EWs as well. Furthermore, it is more interesting to consider some other models consisting of the swapping operators with supersymmetries [61].

Similarly, we consider the following Hamiltonian in terms of the singlet projections

$$H = J \sum_{\langle i,j \rangle} \left(\mathbf{P}_{i,j} - \frac{1}{2s+1} \right) \tag{54}$$

From the proposition II, we can easily prove that $\langle H \rangle \geq 0$ for a separable state, indicating that the Hamiltonian can be viewed as an EW. Any superposition of operators $\tilde{\mathbf{P}}_{i,j} = \left(\mathbf{P}_{i,j} - \frac{1}{2s+1} \right)$ with positive coefficients are EWs as well. Moreover, the

IV. SUMMARY

We have derived the general form of the spin swapping operator for the quantum Heisenberg spin-s systems, and proved that under the partial transposition the general spin swapping operator is equal to the singlet projection operator. For SU(2) invariant bipartite spin-s systems, we also found that the expectation value of the swapping operator is the leading contribution to the negativity. Generalized to the many-body particle states, the expectation values of the swapping and permutation operators can be used as an entanglement witness, which, moreover, in some cases can be used for formulation of necessary and sufficient condition of entanglement. This is a quite important and new mathematical fact, which could be used for the formulation of observable conditions of entanglement in near future.

The authors acknowledged that this research work was finalized when both of us visited the Center for Theoretical and Computational Physics of the University of Hong Kong. G. M. Zhang is supported by NSF-China (Grant No. 10125418 and 10474051). X. G. Wang is supported by NSF-China under grant no. 10405019, Specialized Research Fund for the Doctoral Program of Higher Education (SRFDP) under grant No.20050335087, and the project-sponsored by SRF for ROCS and SEM.

[1] A. Peres, Phys. Rev. Lett. **77**, 1413 (1996).
[2] M. Horodecki, P. Horodecki, and R. Horodecki, Phys. Lett. A 223, 8 (1996).
[3] K. Zyczkowski, P. Horodecki, A. Sanpera, and M. Lewenstein, Phys. Rev. A **58**, 883 (1998); K. Zyczkowski, Phys. Rev. A 60, 3496 (1999). G. Vidal and R. F. Werner, Phys. Rev. A, **65** 032314 (2002).
[4] R. F. Werner, Phys. Rev. A **40**, 4277 (1989).
[5] M. Horodecki and P. Horodecki, Phys. Rev. A **59**, 4206 (1999).
[6] K. G. Vollbrecht and R. F. Werner, Phys. Rev. A **64**, 062307 (2001).
[7] J. Schliemann, Phys. Rev. A 68, 012309 (2003); Phys. Rev. A 72, 012307 (2005).
[8] H. P. Breuer, Phys. Rev. A **71**, 062330 (2005).
[9] H. P. Breuer, J. Phys. A: Math. Gen. **38**, 9019 (2005).
[10] M. A. Nielsen, Ph. D thesis, University of Mexico, 1998, quant-ph/0011036;
[11] M. C. Arnesen, S. Bose, and V. Vedral, Phys. Rev. Lett. **87**, 017901 (2001).
[12] X. Wang, Phys. Rev. A **64**, 012313 (2001); Phys. Lett. A **281**, 101 (2001).
[13] D. Gunlycke, V. M. Kendon, V. Vedral, and S. Bose, Phys. Rev. A **64**, 042302 (2001).
[14] G. Jaeger, A. V. Sergienko, B. E. A. Saleh, and M. C. Teich, Phys. Rev. A **68**, 022318 (2003).
[15] S. Bose and V. Vedral, Phys. Rev. A **61**, 040101 (2000).
[16] G. L. Kamta and A. F. Starace, Phys. Rev. Lett. **88**, 107901 (2002).
[17] K. M. O'Connor and W. K. Wootters, Phys. Rev. A **63**, 0520302 (2001).
[18] D. A. Meyer and N. R. Wallach, quant-ph/0108104.
[19] T. J. Osborne and M. A. Nielsen, Phys. Rev. A **66**, 032110 (2002).
[20] A. Osterloh, L. Amico, G. Falci and R. Fazio, Nature **416**, 608 (2002).
[21] Y. Sun, Y. G. Chen, and H. Chen, Phys. Rev. A **68**, 044301 (2003).
[22] U. Glaser, H. Büttner, and H. Fehske, Phys. Rev. A **68**, 032318 (2003).
[23] L. F. Santos, Phys. Rev. A **67**, 062306 (2003).
[24] Y. Yeo, Phys. Rev. A **66**, 062312 (2002).
[25] D. V. Khveshchenko, Phys. Rev. B **68**, 193307 (2003).
[26] L. Zhou, H. S. Song, Y. Q. Guo, and C. Li, Phys. Rev. A **68**, 024301 (2003).
[27] G. K. Brennen, S. S. Bullock, Phys. Rev. A **70**, 52303 (2004).
[28] R. Xin, Z. Song, and C. P. Sun, quant-ph/0411177.

[29] F. Verstraete, M. Popp, and J. I. Cirac, Phys. Rev. Lett. **92**, 027901 (2004).
[30] F. Verstraete, M. A. Martin-Delgado, J. I. Cirac, Phys. Rev. Lett. **92**, 087201 (2004).
[31] J. Vidal, G. Palacios, and R. Mosseri, Phys. Rev. A **69**, 022107 (2004).
[32] S. Ghose, T. F. Rosenbaum, G. Aeppli, and S. N. Coppersmith, Nature (London) **425**, 48 (2003).
[33] H. Fan, V. Korepin, and V. Roychowdhury, Phys. Rev. Lett. **93**, 227203 (2004).
[34] F. Verstraete, M. A. Martín-Delgado, and J. I. Cirac, Phys. Rev. Lett. **92**, 087201 (2004).
[35] S. J. Gu, H. Q. Lin, and Y. Q. Li, Phys. Rev. A **68**, 042330 (2003).
[36] Y. Chen, P. Zanardi, Z. D. Wang, and F. C. Zhang, quant-ph/0407228.
[37] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev Phys. Rev. Lett. **90**, 227902 (2003).
[38] X. Wang and P. Zanardi, Phys. Lett. A **301**, 1 (2002); X. Wang, Phys. Rev. A **66**, 044305 (2002); Phys. Rev. E **69**, 066118 (2004).
[39] W. K. Wootters, Phys. Rev. Lett. **80**, 2245 (1998).
[40] M. Horodecki, P. Horodecki, and R. Horodecki, Phys. Lett. A **223** l (1996).
[41] B. M. Terhal, Phys. Lett. A **271**, 319 (2000).
[42] M. Lewenstein, B. Kraus, J. I. Cirac, and P. Horodecki, Phys. Rev. A **62**, 052310.
[43] A. Auerbach, *Interacting Electrons and Quantum Magnetism* (Springer-Verlag, New York, 1994).
[44] R. Gilmore, *Lie Algebras and Some of Their Applications* (John Wiley & Sons, New York, 1974).
[45] M. T. Batchelor and M. N. Barber, J. Phys. A **23** L15 (1990); A. Klumper, J. Phys. A **23**, 809 (1990).
[46] M. T. Batchelor and C. M. Yung, in *Proceedings of the Confronting the Infinite Conference* in honour of H. S. Green and C. A. Hust (1994); cond-mat/9406072.
[47] G. V. Uimin, JETP Lett. **12**, 225 (1970).
[48] J. K. Lai, J. Math. Phys. **15**, 1675 (1974).
[49] B. Sutherland, Phys. Rev. B **12**, 3795 (1975).
[50] M. R. Dowling, A. C. Doherty, and S. D. Bartlett Phys. Rev. A **70**, 062113 (2004)
[51] G. Tóth, Phys. Rev. A **71**, 010301(R) (2005)
[52] C. Brukner and V. Vedral, quant-ph/0406040.
[53] L. -A. Wu, S. Bandyopadhyay, M. S. Sarandy, and D. A. Lidar, Phys. Rev. A **72**, 032309 (2005).
[54] P. Hyllus, O. Gühne, D. Bruss and M. Lewenstein, Phys. Rev. A **72**, 012321 (2005).
[55] G. Toth and O. Göhne, Phys. Rev. A **72**, 022340 (2005).
[56] R. A. Bertlmann, K. Durstberger, B. C. Hiesmayr, and P. Krammer, Phys. Rev. A **72**, 052331 (2005).
[57] M. Bourennane, M. Eibl, C. Kurtsiefer, S. Gaertner, H. Weinfurter, O. Gühne, P. Hyllus, D. Bruß, M. Lewenstein, and A. Sanpera, Phys. Rev Lett. **92**, 087902 (2004).
[58] M. Stobiòska and K. Wódkiewicz, Phys. Rev. A **71**, 032304 (2005).
[59] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, 1957).
[60] M. Horodecki, P. Horodecki, and R. Horodecki, preprint, cond-mat/0206008.
[61] F. H. L. Essler and V. E. Korepin, Phys. Rev. B **46**, 9147 (1992); Jan de Boer, V. E. Korepin, and A. Schadschneider, Phys. Rev. Letts. **74**, 789 (1995); F. H. L. Essler, V. E. Korepin, and K. Schoutens, Phys. Rev. Letts. **70**, 73 (1993).